



chain nodes :

17 18

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14

chain bonds :

7-17 10-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13 13-14

exact/norm bonds :

7-17 10-18

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13 13-14

G1:Cl,Br,F,I,CH3,Et,n-Pr,s-Bu,CF2,MeO,EtO,n-PrO,CN

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 17:CLASS 18:CLASS